Generation of Requirements for Simulant Measurements

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Executive Summary

This document provides a formal, logical explanation of the parameters selected for the Figure of Merit algorithm used to evaluate lunar regolith simulant. The objectives, requirements, assumptions and analysis behind the parameters is provided.

From NASA's objectives for lunar simulants a requirement is derived to verify and validate simulant performance versus lunar regolith. This requirement leads to a specification that comparative measurements be taken the same way on the regolith and the simulant. In turn this leads to a set of 9 criteria with which to evaluate comparative measurement. Many of the potential measurements of interest are not defensible under these criteria, for example many geotechnical properties of interest were not explicitly measured during Apollo and they can only be measured *in situ* on the Moon.

A 2005 workshop identified 32 properties of major interest to users (Sibille Carpenter Schlagheck, and French, 2006). Virtually all of the properties are tightly constrained, though not predictable, if just four parameters are controlled. Three: composition, size and shape, are recognized as being definable at the particle level. The fourth, density, is a bulk property.

In recent work a fifth parameter has been identified, which will need to be added to future releases of the Figure of Merit: spectroscopy.

Objectives and Requirements

The Figure of Merit evaluation criteria for lunar regolith simulants was established from an analysis of NASA objectives for the simulant. The Figure of Merit criteria are a series of measurements. These measurements compare quantitatively a sample of regolith and a sample of simulant. This document provides a historical view of why the measurements in the Figure of Merit criteria were selected, why others were not selected, and the consequences of the selection to specific problems of interest for engineering applications.

Table 1: NASA Simulant Objectives

O1	Reproduce characteristics of lunar regolith using simulants.
O2	Produce simulants as cheaply as possible.
O3	Produce simulants in the amount needed.
O4	Produce simulants to meet users' schedules.

This document deals only with the first NASA simulant objective: reproduce characteristics of lunar regolith using simulants. Thus, the following requirement is yielded.

Requirement 1- Verify and validate simulant performance versus lunar regolith.

Analysis of the requirement implied a direct comparison of measurements taken on lunar regolith and measurements on simulant. Simplicity and a desire for high confidence strongly recommended that the same measurements be taken on regolith and simulant. This approach was adopted in the following specification:

Specification 1 – Requirement 1 shall be satisfied by comparison of measurements taken the same way on both regolith and simulants.

Analysis 1

It should be noted that using identical measurements on regolith and simulant is not a necessity. This is a design choice and as such is subject to trade analysis. Permitting the use of non-identical measurements permits greater flexibility. As an example, Apollo program Surveyor scoop measurements might be used to provide a lunar geotechnical value; a different method must be used to evaluate the same value with lunar regolith simulant. Scientifically, this is a common technique, which allows one to take advantage of all the available data in a data-poor situation.

A primary difficulty with this approach is that one needs to have a high degree of confidence that the two different measurements are functionally equivalent within the tolerance of the application. To meet the stated objectives, this is a very difficult constraint. The regolith is not a material with which we have a lot of engineering experience, and the abundant scientific measurements are focused on features which are not perfectly translatable to engineering needs. Defending, or understanding of, the equivalence of two different measurements can be difficult, especially for the non-expert.

Further, there is a general paucity of geotechnical and engineering measurements on the regolith, especially for measurements taken on the Moon. The amount of published data pertaining to geology dwarfs the geotechnical and engineering data. Finally, there is no single sample for which all, or even a majority, of the desired measurements were obtained.

This is a major consideration. Even the most casual survey of the lunar literature shows the regolith varies rapidly and substantially as one moves from any given point. It is a truism that the concept of "average" is useful, but what is processed is always a specific sample. It can be useful to test with average material, but exclusively doing so for an innovative design placed in a high-risk environment is probably not prudent. But, if there is no single sample of the regolith which was measured for all the properties, some concept of average or typical is all that can be used. It was thus concluded that using different measurement techniques on regolith and on simulants was an inherently risky option.

Basic Data

Having stated the requirement, examined the conceptual options, and selected an approach, there are many technical considerations.

Table 2: Design Considerations for Measurements

A. The individual measurements must be	i. agreed on,
	ii. practical to make on both simulant and regolith,
	iii. reproducible,
	iv. of properties that process controls can affect consistently,
	v. functionally or physically meaningful,
	vi. taken in a uniform, standardized manner,
B. Measurements should be as few as technically defensible.	
C. The phenomena measured should be independent.	
D. The phenomena measured should have maximal explanatory power.	

It is desirable for the measurements and underlying phenomena to have intuitive meaning and direct applicability to the users' needs, but this is a design choice and not a demand of the requirement. There is no requirement to provide measurements that match user needs or desires based on their individual backgrounds or training.

Analysis 2

Analysis of the above, known engineering needs, and existing knowledge of the lunar regolith provides the following points.

1. Unless they were measured during Apollo, many of the measurements of interest cannot be known with precision for lunar materials as they would have to be measured *in situ*. This is obviously true for phenomena that are sensitive to precise interactions between aggregates of particles *in situ*, such as bearing strength. While some data for bearing strength exists from Apollo, to state that the bearing strength of any given regolith is known sufficiently to verify and validate a simulant's performance is unreasonable.
2. Any single parameter can be measured in many ways and the method of measurement strongly affects the values determined. Often the correspondence between two methods of measurement is poor.

3. Selecting which method of measurement is used is often contentious, as many specific measurements are made in a specialized way by each individual user. Simulants will be needed for more than a decade, and will be measured by numerous groups with updated equipment.
4. Estimates of the volumes of simulant that will be needed are at best speculative, and production of additional simulant will require repeated precise measurements.
5. Critical measurements should not be limited to a single person or piece of equipment.
6. There is a cost, often very substantial, to making a measurement. A conservative estimate of the number of measurements will have to be made.
7. The average particle size of the lunar regolith is approximately 50 microns.
8. The average grain size is substantially smaller than the average particle size.
9. The regolith has substantial and functionally significant variations on almost any spatial scale of relevance to engineering.
10. There is no standard method for comparison of two mixtures of particulates when the composition, sizes, and shapes of the particles can all vary simultaneously.
11. The materials of interest, regolith and simulants, are geological products. They are not engineered products.
12. The body of knowledge which describes the materials of interest is geology.

Assumptions

A statement of two explicit assumptions made is necessary in addition to the given objectives, derived requirement, stated design considerations, and compiled salient facts.

First, the behavior of the regolith is not uniquely a function of being on the Moon. We are assuming that there is nothing about being on the Moon that changes the physics of materials in manners unknown on Earth. In simple terms, physics is physics.

Second, conceptually one can find two divergent approaches to measurement standards. One is based on a systematic language and requires a framework of integrated concepts, and the other approach is *ad hoc.* Familiar examples of the first approach are standards related to the load-bearing capacity of structural components. These standards use a common terminology, taught in basic physics, and depend on the formal concepts of science. Further, it should be noted that using such measurements frequently requires use of the formal concepts (e.g., bending resistance of a steel beam). In the *ad hoc* approach, a test is created which relates to a property of interest, but the measurement protocols and results cannot be immediately tied to anything else. An example of this approach used in soil

engineering is the Atterberg limit codified in ASTM D4943-08 "Standard Test Method for Shrinkage Factors of Soils by the Wax Method." While very useful in practical applications, it is highly problematic to relate numbers obtained under ASTM D4943-08 to other parameters except by making organized suites of measurements and seeking correlations. First principles are not needed to express or use these measurements.

Both systematic and *ad hoc* methods are commonly used in measurement standards. There are benefits and problems with each approach. The systematic approach has the advantage of explicit ties to basic concepts; such measurements can say something fundamental. It has a disadvantage in that some knowledge of the basic concepts is needed to use or understand the measurements. The *ad hoc* approach has the advantage of directly addressing a specific need. The major disadvantage to the *ad hoc* method is that it is almost useless where broad application in different fields is needed. There is no common framework of basic concepts to guide and inform different uses. An *ad hoc* approach is commonly used within highly specialized and tightly restricted applications; understanding their limitations and their utility frequently depends on considerable technical knowledge. Further, it is common that specialized applications in a field will develop multiple versions of the same *ad hoc* "standard" measurement to suit specific types of problems. It is impractical to rigorously relate the results of one "standard" measurement to another "standard" measurement.

Simulants will be needed by a broad range of users with diverse technical backgrounds who will be using the simulants in unrelated ways. Questions about load-bearing capacity are quite different from questions of air filtration, water filtration, high temperature melting, or movement induced by rocket plume exhaust. Yet all are dealing with the same regolith. **It was therefore assumed that in this case an organized approach to measurement standards was overwhelmingly superior** and probably the only tractable approach. The number of desired *ad hoc* measurements is almost certainly beyond any reasonable budget.

Therefore, a set of measurements was sought which would be based on a systematic language and a framework of integrated concepts. Because the lunar regolith is a geologic material made from broken and melted rock, it was concluded that the source of the most rigorous vocabulary and conceptual framework for this purpose was from the field of geology.

Determination of Measurements

Most people will agree that what the regolith or simulants are made of has bearing on many of the properties of engineering interest. Geologically, the lunar regolith is broken and melted (glass) rock. The individual particles of the regolith are a variable mixture of pieces of rock, pieces of minerals, and pieces of glass (see Table 3 for representative particle composition of lunar highlands regolith). Rocks, of the type relevant to the Moon, are various combinations of minerals and glasses. Glass is a brittle solid that does not show atomic ordering on a scale sufficient to diffract

X-rays. Its composition can in theory be almost anything, but the lunar glasses are dominantly silicate based, because the dominant source materials for the glasses are silicate minerals. To a geologist, lunar rocks are defined in a context of mineralogy.

Mineralogy, of course, is the study of minerals. According to the Glossary of Geology (1974), a mineral is a naturally occurring chemical element or compound having a definite chemical composition and, usually, a characteristic crystal form. One of the subsidiary statements in the definition of mineral is "A naturally occurring, usually inorganic, crystalline substance with characteristic physical and chemical properties that are due to its atomic arrangement." What does the definition mean to an engineer?

First, the natural world does not assemble atoms in geologic solids at random, there is almost always order on very large scales, involving >>10^9 atoms per discrete entity (grain, particle, crystal, etc.). Only certain orders or patterns occur naturally. On Earth less than 5000 such patterns, i.e. minerals, are known, and most of those are extremely rare. Known patterns from the Moon are less than a few hundred (e.g., Frondel 1975). When one examines a pattern, i.e. mineral, one finds the atoms are assembled into an extremely consistent spatial pattern, termed a unit cell. The unit cell is repeated in three dimensions to form a lattice (Figure 1). Within a given lattice, an element can only occupy specific positions. This in turn limits the ratios of the elements within a mineral. For example, the mineral forsterite (Mg_2SiO_4) must have one silicon atom for every two magnesium atoms and four oxygen atoms. Thus, it is the presence of specific minerals in the lunar regolith that restricts its composition. In addition, the elements are going to be locked together in a restricted number of ways.

Table 3: Average proportion of particles in lunar highlands regolith from Apollo 16 core 64001/64002.

Sample 64001/64002 particle type	%
Monomineralic particles	**23.5**
plagioclase	21.5
pyroxene	1.7
olivine	0.2
opaque (oxides and sulfides)	0.1
Crystalline Lithics	**0.7**
Breccia Fragments	**27.9**
Agglutinates	**40.0**
Glass	**7.8**
Total	**100.0**

Data are summarized and averaged from Basu and McKay (1984) and Houck (1982).

Noted in the subsidiary statement to the definition of mineral is the fact that a mineral will have characteristic, i.e. specific, physical and chemical properties. Thus, a forsterite crystal from the Moon must have the same hardness, magnetic susceptibility, dielectric constant, chemistry, strength, melting point, or any additional property of a forsterite crystal from Earth. This is a very tight constraint on the engineering performance of both regolith and simulants.

To the extent lunar regolith is made of minerals and the performance of

the regolith is controlled by the minerals, then simulant with the same mineralogy will replicate the behavior of the regolith.

This constraint raised questions: 1) to what extent is the regolith made of minerals, and 2) to what extent is the performance of the regolith controlled solely by the minerals? The first question has been answered by numerous studies of regolith samples obtained by Apollo astronauts (Table 3). The regolith is effectively a mixture of glasses and minerals. Therefore, mineralogy strongly constrains the performance of regolith and simulants. It was also realized during these studies that the number of minerals on the Moon compared to Earth is actually small, and that fewer than 20 minerals could describe >99% of the regolith. Further, most of the 20 minerals are common terrestrial minerals.

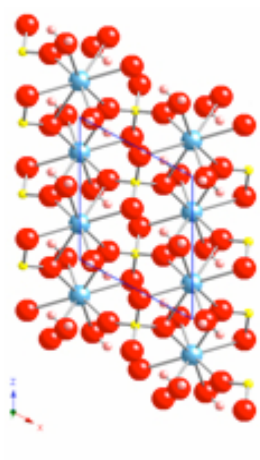

Figure 1: Model of the mineral gypsum ($CaSO_4 \cdot 2H_2O$). Note repetition of the structural elements.

Due to the fact that the word "mineral" does not adequately describe the constituents of the lunar regolith, the word "particle" is used. A particle is hereby defined as a solid entity which, in concept, could be separated from other particles without breaking chemical bonds, either surface to surface or lattice. A grain is a physically distinct subset, typically crystalline, of a particle.

The second question, to what extent are the properties of the regolith controlled by the mineralogy, was initially very difficult. Any answer would require knowledge of all the ways the simulant might be used and all the interactions of the simulant with the equipment; this was functionally impossible. One approach to addressing this problem was to ask experts to recommend what properties might be common to many needs and sufficient to permit adequate testing of components and systems bound for the Moon. This was done in a workshop held in Huntsville in January, 2005 (Sibille et al., 2006). At the workshop, an effort was made to tabulate properties needed to understand engineering interactions with the regolith. The result was a list of 32 properties – too long to be economically practical. Further, many of the implied measurements violated one or more items in Table 2.

An observation was made upon examination of the list from the 2005 workshop. If one understands what controls many of the properties of interest in addition to mineralogy, only a few factors are important. These were informally titled as follows:

1) minerals,

2) glass,

3) rocks,
4) aggregations of disparate materials in single particles,
5) mechanical structures within a grain or particle,
6) relationships between grains,
7) the size of the particles,
8) the shapes of the particles, and
9) how the particles are packed together.

A critical realization was made at this stage.

When dealing with mixtures of particles, practical treatments of behavior may be forced, due to complexity, to deal with measurements of the collection; but their theoretical understanding is very commonly, if not always, founded in the behaviors of individual particles! There is commonly an implicit assumption that if the particles could be understood, the property of interest would be deterministic. By corollary if the particles are reproduced exactly, the observed behavior would be reproduced exactly!

It was also noted that factors one through four concern particle composition. Factors five through eight are geometric attributes of individual grains or particles. The last factor addresses an emergent property that arises from collections of particles.

Mineralogy has already been discussed. There are subtleties which have not been discussed, such as the mineralogy of solid solutions, the distribution of trace elements, and lattice strains due to mechanical and chemical phenomena. The logic used to select a subset of the lunar minerals has not been discussed, but these are clearly secondary or tertiary to a statement that mineralogy is a powerful tool in reproducing lunar regolith.

Background knowledge of each of the other factors is also necessary in order to understand the applicability and limitations of the corollary above.

Glass is of major importance; it can be more than 50% of the total mass of the regolith. In theory it could be made from anything found on the Moon, but it typically has a restricted compositional range. It is produced by only two methods, meteor impacts and volcanism. Therefore, most of the glass will typically have a relatively narrow range of mechanical and chemical properties, especially compared to the minerals. The conclusion was reached that it would be sufficient to measure the abundance of glass to characterize the simulant. As long as the glass composition was roughly similar to that of the rest of the simulant, detailed glass chemistry was not needed.

Rocks are simple collections of grains. The grains can be all one mineral or combinations of minerals. Rocks can also incorporate glasses. Many of the particles in the regolith are fragments of rocks. Rocks do not behave the same way as particles made up of single minerals or glass. The differences are reasonably well understood and are often due to the type of rock. It was therefore reasonable to incorporate a measure of the abundance of rocks by specific type. This was a simplifying assumption, and to a limited extent helped deal with the next two points.

Aggregations of materials in a single particle, such as those found in the lunar regolith, are very difficult to replicate. For this work, "rock" could be considered a special case of such particles. However, it is very simple geologically to treat "rocks" as discrete constituents of the regolith. Therefore, it was decided to restrict consideration of "aggregations" to the subset of particles in the regolith for which there is no natural, terrestrial analog. The most well known "aggregations" on the lunar surface are agglutinates. These are aggregate particles composed of particles welded together by spatter glass. The glass of agglutinates contains spheres or globules of metallic iron which are frequently approximately 30 μm in diameter. Agglutinates can comprise up to 60% of selected regolith. Many regolith particles also have rims composed of glass layers a few nanometers thick; these contain small globules of metallic iron. The rims are presumed to be directly deposited from the vapor phase. The abundance of these rims in lunar regolith is currently unknown.

Agglutinates and the vapor deposited rims would certainly have impacts on engineering performance. Unfortunately, there was no language to quantitatively describe them, or any standard methods to measure them. This makes it very difficult to have quantitative measures, which are necessary if one is to satisfy Requirement 1. There was also no mechanical or chemical data on the behavior of lunar agglutinates. Finally, no one was attempting to reproduce the vapor deposited rims, which were very poorly characterized and difficult to study. The decision was made that agglutinates had to be accounted for in some way and the rims could, at least initially, be ignored. How to define, characterize, and count agglutinates was a problem delayed for further consideration.

The first four of the nine factors: mineralogy, glass, rocks, and aggregations, define what the particles are made of, in other words, the particle's composition. In a geologic sense the only things known in the regolith which fall outside these four are the vapor deposited rims.

The mechanical structures within a grain or particle include things like lamellae (alternating crystals of two related compositions that often appear as stripes) and disruptions of the original grain (such as broken grains). There is no standardized way to express these features, no accepted way to measure these features, and no data on how common these features are. No data exists to describe how these features affect anything. Reason suggests these features will have some bearing on the strength of individual particles, but if the particles mechanically fail then they can be treated as discrete particles. It was therefore decided this feature would have to be ignored for measurements, but a caveat would be associated with them.

It was assumed that, at present, this could be a substantial problem or limitation only when considering particles bigger than approximately one centimeter.

A similar situation exists for relationships between grains within a particle. There are attempts in various literatures to deal with this consideration, but there is no standardization and the affects of grain-to-grain relationships can be very complex. As with features within a grain, it was therefore decided this feature would have to be ignored for measurements, but a caveat would be associated with them. It was anticipated this would be a substantial problem or limitation when considering techniques to beneficiate the regolith, where grain to grain relationships are extremely important. There are other possible situations where grain-to-grain relationships are important, but the judgment was made that the engineering sophistication necessary for such things was well in the future for lunar applications.

If something cannot be measured in a standardized way, and there is no standard language to describe it, and its impact is likely to be relatively minor compared to other things, prudent management of resources and time suggests ignoring the effect, at least initially. Thus, the effects of mechanical structures within grains and particles and the relationships between particles would not be considered in the first generation of standard measurements.

Particle size is intellectually an easy concept. Definition, however, is quite difficult. It becomes a question of how size is measured. A cursory examination of literature about the regolith showed the following: 1) the size range of particles does not show discrete limits, which is not analogous to terrestrial, geologic materials; 2) the particle size range in samples easily goes from multi-centimeter to sub-micron, which is five orders of magnitude; 3) there are at least ten discrete minerals, rocks, and agglutinates that are substantial constituents of the regolith; and 4) except by hand, there are no practical technologies to measure an individual particle's size along with any other property. Consideration of the number of measurements needed to characterize a size distribution given the number of constituents led to the conclusion that at least 10^5 discrete values would be needed for each sample of regolith or simulant evaluated. It was therefore decided that knowledge of each individual particle's size, along with its composition, was not practical, but the distribution of sizes could be obtained for the regolith or simulant as a whole. It would be necessary, at least initially, to assume the size distribution for the whole would be representative of the size distribution of each constituent.

It should be noted that the assumption of identical size distributions was not necessary for the Figure of Merit software. It was relatively straight forward to write the code such that when component specific size data becomes available it will transparently override the assumption of a common size distribution.

A question was asked about the significance and likely impact of the assumption of identical size distribution of each constituent. There is no clear way to quantitatively evaluate this. There is data which suggested some variation in

composition with size, but the differences are not major and informed judgment suggests they are not large enough, compared to other factors, to merit concern at the beginning.

The assumption of uniformity in shape is also used because shape is an easy concept that is hard to measure. Useful values require thousands of measurements, and measurements of individual particles cannot be linked to the particle's composition.

Each point discussed above deals with individual particles. There are, however, many phenomena of interest to engineers that involve how multiple particles interact (e.g., shear strength). Is it necessary to know the size, shape, composition, and spatial orientation of each particle to understand the behavior of the bulk? In almost all, if not all, cases it is not, if two assumptions can be made – random and uniform distributions. In other words, are there biases in size, shape, composition, or orientation which are functions of spatial location? There is little data on the regolith showing preferential orientation of particles (e.g., Mahmood et al., 1974), and there is no data showing broad scale sorting of size or shape. Visual inspection of the regolith shows no apparent preferences. Compared to Earth, this is extremely unusual. There is spatial variation in composition. The mare are clearly different compared to the highlands. The surface commonly has more agglutinates. In contrast, within a single Apollo sample there appears relatively little ordering of composition, at least compared to terrestrial materials. Therefore, it is likely that an assumption of uniform, internal randomness to each sample is not unreasonable.

Having established that randomness and uniform distributions are reasonable assumptions, what measure or measures are needed to characterize the relationships between particles? Only one: packing density. If the specific gravities of the constituents are known, the size and shape distributions are known, and the particles are randomly and uniformly distributed, the only variable left is the tightness of packing of the particles.

At this point, the objectives and consequent requirement have directed attention to basically four parameters: composition, size distribution, shape distribution and density. The numerous assumptions made are known to be robust and are based on available data, common practice, and fundamental understandings.

There are things clearly not explicitly covered by this approach. For example, magnetism is not well handled and is very problematic to reproduce. Nonetheless, magnetism is important and how well it is described depends on what causes the magnetism. If it is derived from specific minerals, it is likely to be well described. If it is due to the agglutinates, it is likely to be well described. If it is due to something else, it is not likely to be well described. Another thing, not recognized as important at the time, is spectral properties: reflectance, transmittance, emission. For this there is substantial data on the lunar materials. As with magnetism, how well it is handled depends on what causes it. If it is dominated by agglutinates and other elements of composition, it is likely to be handled well. Otherwise, it will not be handled well.

Some final notes are in order. First, there are things in terrestrial materials that are not present in studied lunar regolith (e.g., hydrous alteration phases). Simulant producers and users must be aware of this fact, and must consider it during analysis. The impact of these differences is as varied as the differences themselves.

Even though the numbers of parameters to be measured are very few and quite simple, there are serious technical hurdles to getting the measurements. Commonly, these problems derive from the extremely fine average particle size of the regolith. It is daunting to consider how hard it would be to make even more specialized measurements when common, ordinary measurements are so difficult.

Last, the reduction to just four basic parameters must be recognized as just a way station, sufficient to start. The parameters selected are clearly able to robustly <u>constrain</u> the performance of simulant with respect to regolith, though they do not permit <u>prediction</u> of behavior.

Spectroscopy

Addendum of May 30, 2010

In the spring of 2010 the impact of the lunar regolith's reflectance, absorption, transmittance and emission of EM radiation was identified as a significant consideration for thermal system design.

As stated in Table 2 there are several considerations any measurement proposed for a figure of merit should meet. Definitions of the relevant measures are well understood in the remote sensing communities. Appropriate and necessary measurement can be obtained for both the Moon and the simulants. Existing process controls clearly are sufficient to obtain reproducible spectral behavior. The existing simulants vary substantially in their albedos. This variation is stated to be highly significant for design purposes. Spectral measurements, while subtly difficult, are commonly done in highly a reproducible manner with good comparability between labs. The number of measurements required could be as low as one and is not likely to exceed three. The variation in albedo is not obviously and definitively controlled by one or more of the other parameters. Spectroscopy is one of the most powerful tools in modern science. It is used in virtually every field because the data are extremely informative. Spectroscopy, in the general sense, clearly satisfies the considerations for inclusion.

With future development a Figure of Merit will probably need to be defined for spectroscopy.

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